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Molecular dynamics studies of the sputtering of divertor materials

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Abstract

We use molecular dynamics (MD) simulations to study two important erosion processes of divertor materials, namely the chemical sputtering of carbon by hyperthermal deuterium and the self-sputtering of W by redeposited atoms. Although it is generally accepted that MD simulations can provide a good qualitative description of far-from-equilibrium processes, such as irradiation-induced cascades, we show that also good quantitative agreement with experiments is obtained. We further show that the chemical sputtering yield of carbon is reduced by Si doping at impact energies $\leqslant 20$ eV. Significant carbon sputtering is still observed for both undoped and doped structures at 5 eV. Silicon sputtering is negligible at all impact energies studied. For W self-sputtering, sputtering yields higher than one are observed at $\geqslant 1$ keV for normal incidence and at $\geqslant 500$ eV for 20° off-normal incidence.

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1. Introduction

A central issue in the performance of the next-step fusion device ITER is the erosion of the plasma-facing components (PFCs), most importantly the divertor structures [1,2]. Several divertor material candidates have been considered during the last decades in view of their erosion rates under bombardment by plasma particles and impurities, as well as their thermomechanical properties. The ITER design features carbon in the high heat flux parts and tungsten in the other parts of the divertor.

High chemical sputtering yields by hydrogenic species, at energies as low as a few eV [3,4] reduce the lifetime of the carbon PFCs, and lead to codeposition with tritium. There is intense research on the enhancement of carbon-based PFC materials by doping (for an overview, see [5]). One of the dopant candidates is silicon. Carbon materials doped with Si up to 10 at.% have shown excellent plasma-facing properties and reduced carbon sputtering yields [6–9].

The erosion rates of tungsten by hydrogenic particles at fusion-relevant energies are extremely low [10,11]. However, the self-sputtering yields by redeposited W atoms are orders of magnitude higher. Depending on the impact angle, the W self-sputtering yields can be higher than one at energies of several hundreds of eV's [10–12], and may result in net erosion of the PFCs.

The actual conditions in the fusion devices during operation, i.e. the presence of all the erosion mechanisms and impurity species simultaneously, are hard to realize in laboratory experiments. In view of detached divertor plasmas, with electron temperatures $\leqslant 5$ eV, the low impact energies and extremely high flux densities of the hydrogenic species require extrapolation outside the

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measured laboratory data. On the other hand, plasma simulators can study the interactions between the plasma and material surfaces, but the determination of net erosion yields is extremely difficult due to the redeposition of eroded species.

We use molecular dynamics (MD) simulations to study the erosion of the divertor materials C and W. We show that the chemical sputtering of carbon by low-energy ($\leqslant 20$ eV) D irradiation is reduced by Si doping. Carbon sputtering yields of the order of 10^{-3} are still observed at 5 eV. The self-sputtering of tungsten by redeposited W atoms is studied in the energy range 150–1000 eV. In both cases our results agree well with experimental data, showing that MD simulations can give reliable yield estimates on the sputtering of PFC materials.

2. Simulation method

In the MD method [13,14] the motion of a system of atoms is followed by iteratively solving the equations of motion for each atom. The atom velocities are derived from force models, which range from extremely time-consuming quantum-mechanical to fast empirical formulations. Contrary to simulations based on the binary collision approximation, MD simulations can take into consideration the atomic structure of the irradiated sample, many-body collisions, and chemical bond forming and breaking. As our method of simulating irradiation events has been described in detail elsewhere [15,16], we outline here only the central aspects of our simulations.

In both cases studied, we considered irradiation at 300 K. For simulations of the chemical sputtering of carbon, the Si–C–H potential by Beardmore and Smith [17] was used. We created several sample surfaces of deuterated carbon (D/C $\sim$ 0.4). As the surface of carbon PFCs eventually amorphize [18], the surfaces were created from a random network of C, Si and D atoms. The bonding structure was optimized with annealing and pressure scaling simulations (see e.g. Ref. [16]). In the case of Si-doped carbon we considered a homogeneous distribution of Si atoms with a $\mathrm{Si}/(\mathrm{Si}+\mathrm{C})$ ratio of 0.1. Several simulation cell surfaces of undoped and Si-doped carbon were used. The sputtering yields were then taken as the average of the sputtering yields of the individual surfaces.

For the W self-sputtering simulations we employ a modification of the Finnis–Sinclair potential [19] by Ackland and Thetford [20], which has been augmented by a repulsive potential [21] at short interatomic distances. We considered self-sputtering of W(0 0 1) surfaces by single redeposited atoms. Off-normal impact angles of $\theta = 0°$ and 20°, and impact energies between 100 and 1000 eV were used.

3. Results and discussion

3.1. Sputtering of Si-doped carbon

The sputtering of carbon structures by hydrogenic species at low ($\leqslant 30$ eV) irradiation energies can be explained by a mechanism we call *swift chemical sputtering* [22,23]. The ejection of small molecular species from Si-C-D networks is due to the penetration of an impinging atom between two C/Si atoms forming a covalent bond. The bonded atoms are then forced apart, resulting in bond rupture.

The sputtering yields of undoped and Si-doped carbon by D irradiation are shown in Fig. 1. It is seen that the carbon sputtering yields from the Si-doped surfaces are lower throughout the energy range. This reduction is most pronounced at 5 eV ($\sim$35%). As in our previous studies [16,22,24], carbon was mainly sputtered in small CD_x and $\mathrm{C}_2\mathrm{D}_x$ species. Silicon sputtering was only observed at 20 eV, with a yield of $\sim 10^{-4}$.

It is known that the literature values on carbon sputtering yields by low-energy hydrogenic ions have a wide scatter (see Refs. [8,25–31]). This scatter is due to different types of irradiated samples, and the use of different molecular projectiles and methods of determining the sputtering yields. However, it has been well established that carbon-based materials in general have sputtering yields of the order of 10^{-3}–10^{-2} at D impact energies $\sim$10 eV. Our modeling now predicts that no threshold of sputtering is seen at energies down to 5 eV,

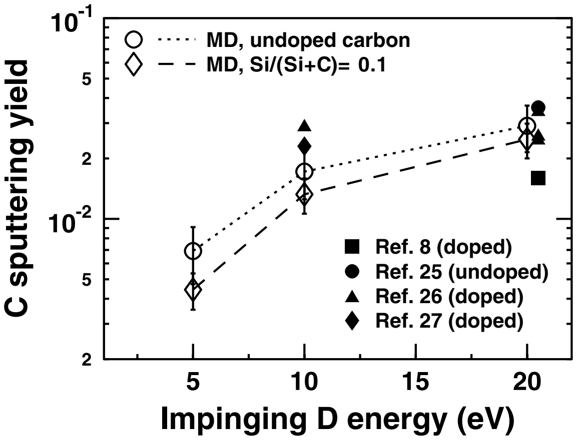

Fig. 1. Carbon sputtering yields for undoped (open circles) and 10 at.% Si-doped (open diamonds) carbon by deuterium. Experimental data for graphite [25] (solid circles) and 10 at.% Si-doped carbon [8,26,27] (other solid symbols) are also shown. At 20 eV the experimental data have been slightly displaced horizontally in order to facilitate the comparison. The MD data for 20 eV are from Ref. [33].

where the yields are still of the order of 10^{-3} (see also Ref. [16]).

3.2. W self-sputtering

Tungsten self-sputtering yields for off-normal impact angles $\theta = 0°$ and 20° are shown in Fig. 2. It is seen that a good agreement between the experiments [12,32] and our modeling is obtained at energies between 300 and 1000 eV. At lower energies, however, deviation from experimental values for the case of normal incidence is seen. A likely reason is that in experiments polycrystalline samples are used, whereas in our modeling we consider only the irradiation of the (0 0 1) surface of W. In both Refs. [12,32] sputtering yields calculated with analytical models and TRIM.SP calculations were also lower than the experimental data at energies below ~300 eV. It was suggested [12] that the oxidation of the sample surfaces results in enhanced reflection of the incident ions. Since the sputtering yields in both sets of experiments were measured with the mass loss method, this would lead to higher sputtering yields. In our simulations no reflection of the incident atoms was observed below an impact energy of 500 eV at normal incidence.

For fusion devices, the most important issue with W self-sputtering is determining the energy range where the sputtering yield is below one. In this energy range there is no possibility of runaway erosion of the sample. Hence, the lifetime of the PFCs is not shortened. For normal incidence it is seen that at energies <1 keV the sputtering yields remain below one. For $\theta = 20°$, the sputtering yields are quite high in comparison with the case of normal incidence and the yield is below one only at energies <500 eV.

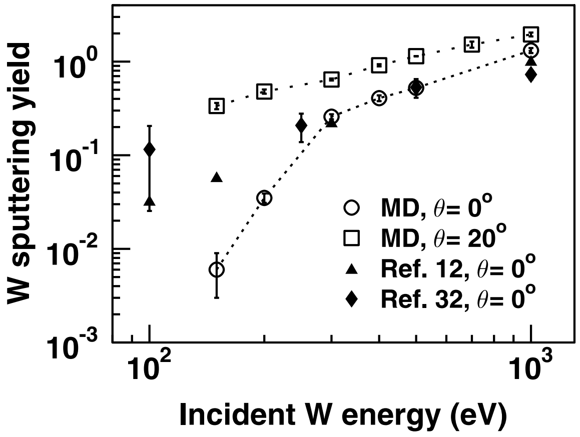

Fig. 2. Self-sputtering yields of W for off-normal impact angles of 0° (open circles) and 20° (open squares). Experimental data for normal incidence [12,32] are also shown. Some of our data are from Ref. [34].

4. Conclusions and outlook

We have shown that the MD method is a useful tool for studying the erosion of divertor materials. For carbon materials, it was shown that Si doping reduces the chemical sputtering of carbon at energies $\leqslant 20$ eV. Sputtering yields of the order of 10^{-3} were still observed at 5 eV. Although in this case a quantitative comparison with experiments is difficult to make due to a wide scatter in the experimental data, a good overall agreement was obtained.

Tungsten self-sputtering was studied in the energy range 150–1000 eV for steep impact angles. In this case, a good agreement with experiments was also obtained.

For divertor material erosion, MD simulations can give reliable quantitative yield estimates also for conditions that are hard to tackle experimentally. These include a wide range and combinations of bombarding species (including tritium) and energy distributions corresponding to the sheath acceleration at different electron temperatures. The simulations on the atomic scale could be coupled to larger scale Monte Carlo simulations for more accurate results on the PFC erosion and redeposition.

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